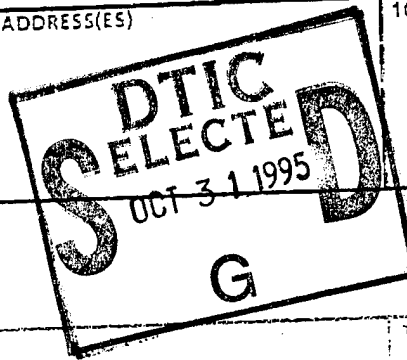


REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503.

1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED FINAL REPORT 01 June 1992 - 31 May 1995
4. TITLE AND SUBTITLE (AASERT-91) Research on Nucleation of II-VI/III-V Semiconductor Heterojunctions		5. FUNDING NUMBERS XXXXXX 3484/S3 61103D AFOSR-TR-95 0688
6. AUTHOR(s) Professor Otsuka		
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Purdue Research Foundation West Lafayette IN 47907-0199		
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) AFOSR/NE 110 Duncan Avenue Suite B115 Bolling AFB DC 20332-0001		10. SPONSORING/MONITORING AGENCY REPORT NUMBER F49620-92-J-0288
11. SUPPLEMENTARY NOTES		
12a. DISTRIBUTION/AVAILABILITY STATEMENT APPROVED FOR PUBLIC RELEASE: DISTRIBUTION UNLIMITED		



13. ABSTRACT (Maximum 200 words)

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19951027 099

DTIC QUALITY INSPECTED 8

14. SUBJECT TERMS		15. NUMBER OF PAGES	
		16. PRICE CODE	
17. SECURITY CLASSIFICATION OF REPORT UNCLASSIFIED	18. SECURITY CLASSIFICATION OF THIS PAGE UNCLASSIFIED	19. SECURITY CLASSIFICATION OF ABSTRACT UNCLASSIFIED	20. LIMITATION OF ABSTRACT UNCLASSIFIED

Final Technical Report
AASERT Grant No. F49620-92-J-0288
(6/1/92-5/31/95)
Research on Nucleation of II-VI/III-V Semiconductor Heterojunctions
Principal Investigators: R. L. Gunshor and N. Otsuka

Two studies were carried out in this program. The first one is molecular dynamics (MD) simulations of MBE growth of ZnSe, and the second one is the analysis of phase separation of ZnSe based alloy epilayers.

One study involved molecular dynamics simulations based on the Lennard-Jones-Axilrod-Teller (LJAT) potential model [1]. Using a set of interatomic potentials based on thermodynamic data and crystal structure data, the atomic configurations in the (110) surface of ZnSe was simulated and compared with experimentally observed surface structure [2]. Excellent agreement was obtained between experimental and calculated parameters. The atomic configuration in the Se-terminated (100) surface was also simulated. The simulations yielded a (2x1) dimer structure, agreeing with the observations, but at present no experimental data are available for quantitative examinations. The result of the study suggested that these interatomic potential models of ZnSe can be used for MD studies of elementary processes of homoepitaxial growth of ZnSe by MBE.

At the next stage of this MD simulation study, we tried to develop the interatomic potentials of Ga_2Se_3 and Zn_3As_2 in order to investigate the nucleation process of ZnSe on (100)GaAs. It was concluded that the LJAT potential model is too simple to describe those compound structures.

The second part of the program involved an investigation of phase separation in $\text{ZnSe}_{1-x}\text{S}_x$ and $\text{Zn}_{1-y}\text{Mg}_y\text{Se}_{1-x}\text{S}_x$ epilayers. During the course of the transmission electron microscope (TEM) analysis of laser structures grown by MBE, we observed phase separation in a number of ternary and quaternary layers [3]. The phase separation occurred nearly along the [011] direction in the (100) epilayers. All observed quaternary epilayers with sulfur concentrations greater than $x=0.2$ exhibited strong phase separation. About one half of the $\text{ZnSe}_{1-x}\text{S}_x$ layers were found to have phase separation. The X-ray microanalysis has shown that the phase separation is described as the formation of S-rich and S-deficient bands.

The only report of experimental studies of the $\text{ZnSe}_{1-x}\text{S}_x$ system suggests that this alloy is completely miscible at 900°C. We have examined if this observed phase separation can occur under the equilibrium condition by using the delta lattice parameter (DLP) model. According to this model, the $\text{ZnSe}_{1-x}\text{S}_x$ system is expected to be completely miscible at the temperatures used in the MBE growth, suggesting that the observed phase separation, i.e., compositional modulation, is a kinetically driven phenomenon. The observation that TEM images of [01 $\bar{1}$] cross-sectional samples of epilayers having phase separation exhibit a wavy surface structure, and also that the period of the wavy surface structure exactly matches that of the compositional modulation, suggests a possible mechanism for the compositional modulation as each valley matches a sulfur-rich band. Sulfur the lowest sticking coefficient of any specie and, hence, is likely to attach more efficiently to step or kink sites during the MBE growth. The wavy surface structure results in a periodic variation of the step density; the step density decreases at the hill and increases at the valley region. The wavy surface structure, therefore, may result in a nonuniform incorporation of sulfur atoms and, hence, lead to the compositional modulation.

- [1] J.F. Egler, MS. Thesis, Purdue University, December (1993).
- [2] C.B. Duke, A. Paton, A. Kahn, and D.W. Tu, J. Vac. Sci. Technol. B2, 366 (1984).
- [3] G.C. Hua, N. Otsuka, D.C. Grillo, J. Han, L. He, and R.L. Gunshor, J. Cryst. Growth, 138, 367 (1994).

Student supported by this program: J. F. Egler

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